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DIFFUSION CONSTANT OF PROTEINS IN BIOMEMBRANES

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In a simple model of the diffusion of macromolecules in a biomembrane, a lipid bilayer can be regarded as an infinitely thin sheet of viscous fluid. These macromolecules move laterally in the fluid sheet as Brownian particles due to the forces exerted by the surrounding lipid molecules. In a two-dimensional fluid, however, the hydrodynamics is not very simple. Once we neglect the convective acceleration term in the Navier-Stokes equation, we face the Stokes paradox. Even if the convective acceleration term is partly included in the Oseen approximation, we are confronted with the breakdown of the linear relation between the velocity and the drag force acting on a macromolecule.

Actually, the Stokes paradox does not exist in real biomembranes. This is because a lipid bilayer is not an isolated fluid but surrounded by adjacent water. Hence the total momentum of the two-dimensional fluid membrane is *not* a conserved quantity and can leak into the surrounding water being a three-dimensional fluid. On the basis of these considerations, Izuyama and coworkers proposed the following two-dimensional hydrodynamical model where the momentum leak is simply represented by a phenomenological relaxation parameter Γ [1, 2];

$$\rho\frac{\partial \boldsymbol{v}(\boldsymbol{r},t)}{\partial t} - \eta\nabla^2\boldsymbol{v}(\boldsymbol{r},t) + \mathrm{grad}\ p(\boldsymbol{r},t) + \Gamma\boldsymbol{v}(\boldsymbol{r},t) = \boldsymbol{F}(\boldsymbol{r},t), \tag{1}$$

supplemented by the incompressibility condition div $\boldsymbol{v}(\boldsymbol{r},t) = 0$. In the above, $\boldsymbol{v}(\boldsymbol{r},t)$ and $p(\boldsymbol{r},t)$ are the velocity and pressure, ρ and η are the density and dynamic viscosity of the lipid membrane, respectively. $\boldsymbol{F}(\boldsymbol{r},t)$ represents any external force acting on the membrane, including Brownian forces.

First we shall consider the case where the protein is modelled by a linear polymer chain. The conformation of a single chain is represented by the set of $(N+1)$ position vectors $\{\boldsymbol{R}_n\} \equiv (\boldsymbol{R}_0, \ldots, \boldsymbol{R}_N)$. Within the preaveraging approximation, the diffusion constant of a polymer chain with an effective bond length b can be calculated as [3]

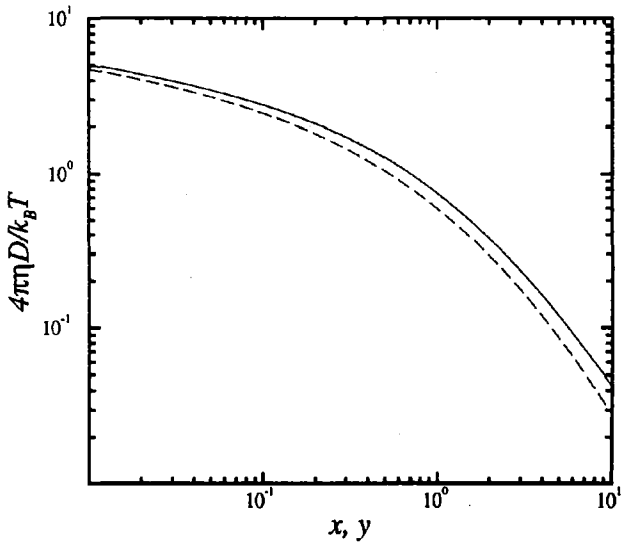
$$\frac{D_p}{k_BT} = \frac{1}{4\pi\eta}\frac{1}{x^4}\left[(1+x^2)(2\log x + \gamma) - x^2 - \exp(x^2)\mathrm{Ei}(-x^2)\right], \tag{2}$$

where $x \equiv (b^2N/4\xi^2)^{1/2} \equiv R_p/\xi$ (R_p being the Gaussian polymer size and $\xi = (\eta/\Gamma)^{1/2}$ the screening length). $\mathrm{Ei}(-z)$ is the exponential integral function defined by $\mathrm{Ei}(-z) = -\int_z^\infty dt e^{-t}/t$ and γ is Euler's constant $\gamma = 0.5772\cdots$. In the weak coupling limit ($x \ll 1$), Eq. (2) reduces to $D_p/k_BT \approx (1/4\pi\eta)(\log\xi/R_p + 3/4 - \gamma/2)$. In the strong coupling limit ($x \gg 1$), on the other hand, it gives $D_p/k_BT \approx (1/4\pi\eta)(\xi/R_p)^2$, neglecting a logarithmic correction.

Next we consider the case where the protein is represented by a cylinder of radius R_c. By using the "induced force method", the translational diffusion constant is calculated as

$$\frac{D_c}{k_BT} = \frac{1}{4\pi\eta}\left(\frac{y^2}{4} + \frac{yK_1(y)}{K_0(y)}\right)^{-1}, \tag{3}$$

where $y = R_c/\xi$, $K_0(z)$ and $K_1(z)$ are the modified Bessel functions of the second kind of order zero and one, respectively. In the weak coupling limit ($y \ll 1$), Eq. (3) becomes $D_c/k_BT \approx (1/4\pi\eta)(\log 2\xi/R_c - \gamma)$, while in the strong coupling limit ($y \gg 1$), we find $D_c/k_BT \approx (1/\pi\eta)(\xi/R_c)^2$. The dimensionless diffusion constants $4\pi\eta D_p/k_BT$ (solid curve) and $4\pi\eta D_c/k_BT$ (dashed curve) are plotted in the following figure versus $x = R_p/\xi$ and $y = R_c/\xi$, respectively.



One of the advantages of the "induced force method" is that we can treat many bodies motion taking the hydrodynamic interaction to some extent. Let us denote the position of i-th cylinder as $\boldsymbol{R}_i$ and the force exerted by the fluid on the j-th cylinder as $\boldsymbol{K}_j$. Then the mobility tensor $\boldsymbol{\mu}_{ij}$ is defined by $d\boldsymbol{R}_i/dt = -\sum_{j=1} \boldsymbol{\mu}_{ij} \cdot \boldsymbol{K}_j$. According to the lowest order multipole expansion and taking the weak coupling limit, we obtained for $i = j$ as $\boldsymbol{\mu}_{ii} = (1/4\pi\eta)K_0(y)I_0(y)\mathbf{1}$, where $\mathbf{1}$ is the unit tensor and $I_0(z)$ is the modified Bessel function of the first kind of order zero. For $i \neq j$, on the other hand, we have

$$\boldsymbol{\mu}_{ij} = \frac{1}{2\pi\eta}\left[\left\{K_0(R_{ij}/\xi) - \frac{\xi}{R_{ij}}K_1(R_{ij}/\xi)\right\}\mathbf{1} + \hat{\boldsymbol{R}}_{ij}\hat{\boldsymbol{R}}_{ij}K_2(R_{ij}/\xi)\right] I_0^2(y), \tag{4}$$

where $\boldsymbol{R}_{ij} = \boldsymbol{R}_j - \boldsymbol{R}_i$, $\hat{\boldsymbol{R}}_{ij}$ is the unit vector parallel to $\boldsymbol{R}_{ij}$ and $K_2(z)$ is the modified Bessel function of the second kind of order two. Details of the calculation will be published elsewhere.

References

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